What is claimed is:

1. A molecule or molecular complex comprising at least a portion of an *S. aureus* NAD synthetase or NAD synthetase-like substrate binding pocket, wherein the substrate binding pocket comprises the amino acids listed in Table 3, the substrate binding pocket being defined by a set of points having a root mean square deviation of less than about 1.1Å from points representing the backbone atoms of said amino acids as represented by the structure coordinates listed in Table 1.

2. The molecule or molecular complex of claim 1, wherein the substrate binding pocket comprises the amino acids listed in Table 4.

3. The molecule or molecular complex of claim 1, wherein the substrate binding pocket comprises the amino acids listed in Table 5.

4. A molecule or molecular complex that is structurally homologous to an *S. aureus* NAD synthetase molecule or molecular complex, wherein the *S. aureus* NAD synthetase molecule or molecular complex is represented by at least a portion of the structure coordinates listed in Table 1.

5. A scalable three-dimensional configuration of points, at least a portion of said points derived from structure coordinates of at least a portion of an *S. aureus* NAD synthetase molecule or molecular complex listed in Table 1 comprising at least one of an *S. aureus* NAD synthetase or NAD synthetase-like substrate binding pocket.

6. The scalable three-dimensional configuration of points of claim 5, wherein substantially all of said points are derived from structure coordinates of an *S. aureus* NAD synthetase molecule or molecular complex listed in Table 1.

7. The scalable three-dimensional configuration of points of claim 5 wherein at least a portion of the points derived from the *S. aureus* NAD synthetase structure coordinates are derived from structure coordinates representing the locations of at least the backbone atoms of amino acids defining an *S. aureus* NAD synthetase substrate binding pocket, the substrate binding pocket comprising the amino acids listed in Table 3.

8. The scalable three-dimensional configuration of points of claim 7, wherein the substrate binding pocket comprises the amino acids listed in Table 4.

9. The scalable three-dimensional configuration of points of claim 7, wherein the substrate binding pocket comprises the amino acids listed in Table 5.

10. The scalable three-dimensional configuration of points of claim 5 displayed as a holographic image, a stereodiagram, a model or a computer-displayed image.

11. A scalable three-dimensional configuration of points, at least a portion of the points derived from structure coordinates of at least a portion of a molecule or a molecular complex that is structurally homologous to an *S. aureus* NAD synthetase molecule or molecular complex and comprises at least one of an *S. aureus* NAD synthetase or NAD synthetase-like substrate binding pocket.

12. The scalable three-dimensional configuration of points of claim 11 displayed as a holographic image, a stereodiagram, a model or a computer-displayed image.

13. A machine-readable data storage medium comprising a data storage material encoded with machine readable data which, when using a machine programmed with instructions for using said data, is capable of displaying a graphical three-dimensional representation of at least one molecule or molecular complex selected from the group consisting of:

(i) a molecule or molecular complex comprising at least a portion of an *S. aureus* NAD synthetase or NAD synthetase-like substrate binding pocket comprising the amino acids listed in Table 3, the substrate binding pocket defined by a set of points having a

root mean square deviation of less than about 1.1Å from points representing the backbone atoms of said amino acids as represented by structure coordinates listed in Table 1; and

(ii) a molecule or molecular complex that is structurally homologous to an *S. aureus* NAD synthetase molecule or molecular complex, wherein the *S. aureus* NAD synthetase molecule or molecular complex is represented by at least a portion of the structure coordinates listed in Table 1.

14. A machine-readable data storage medium comprising a data storage material encoded with a first set of machine readable data which, when combined with a second set of machine readable data, using a machine programmed with instructions for using said first set of data and said second set of data, can determine at least a portion of the structure coordinates corresponding to the second set of machine readable data, wherein said first set of data comprises a Fourier transform of at least a portion of the structure coordinates for *S. aureus* NAD synthetase listed in Table 1; and said second set of data comprises an x-ray diffraction pattern of a molecule or molecular complex of unknown structure.

15. A method for obtaining structural information about a molecule or a molecular complex of unknown structure comprising:

crystallizing the molecule or molecular complex;

generating an x-ray diffraction pattern from the crystallized molecule or molecular complex;

applying at least a portion of the structure coordinates set forth in Table 1 to the x-ray diffraction pattern to generate a three-dimensional electron density map of at least a portion of the molecule or molecular complex whose structure is unknown.

16. A method for homology modeling an *S. aureus* NAD synthetase homolog comprising:

aligning the amino acid sequence of an *S. aureus* NAD synthetase homolog with an amino acid sequence of *S. aureus* NAD synthetase (SEQ ID NO: 1) and incorporating the sequence of the *S. aureus* NAD synthetase homolog into a model of *S. aureus* NAD synthetase derived from structure coordinates set forth in Table 1 to yield a preliminary model of the *S. aureus* NAD synthetase homolog;

subjecting the preliminary model to energy minimization to yield an energy minimized model;

remodeling regions of the energy minimized model where stereochemistry restraints are violated to yield a final model of the *S. aureus* NAD synthetase homolog.

17. A computer-assisted method for identifying an inhibitor of *S. aureus* NAD synthetase activity comprising:

supplying a computer modeling application with a set of structure coordinates of a molecule or molecular complex, the molecule or molecular complex comprising at least a portion of an *S. aureus* NAD synthetase or NAD synthetase-like substrate binding pocket, the substrate binding pocket comprising the amino acids listed in Table 3;

supplying the computer modeling application with a set of structure coordinates of a chemical entity; and

determining whether the chemical entity is an inhibitor expected to bind to or interfere with the molecule or molecular complex, wherein binding to or interfering with the molecule or molecular complex is indicative of potential inhibition of *S. aureus* NAD synthetase activity.

18. The method of claim 17 wherein the substrate binding pocket comprises the amino acids listed in Table 3, the substrate binding pocket being defined by a set of points having a root mean square deviation of less than about 1.1Å from points representing the backbone atoms of said amino acids as represented by structure coordinates listed in Table 1.

19. The method of claim 17 wherein determining whether the chemical entity is an inhibitor expected to bind to or interfere with the molecule or molecular complex comprises performing a fitting operation between the chemical entity and a binding pocket of the molecule or molecular complex, followed by computationally analyzing the results of the fitting operation to quantify the association between the chemical entity and the binding pocket.

20. The method of claim 17 further comprising screening a library of chemical entities.

21. A computer-assisted method for designing an inhibitor of *S. aureus* NAD synthetase activity comprising:

supplying a computer modeling application with a set of structure coordinates of a molecule or molecular complex, the molecule or molecular complex comprising at least a portion of an *S. aureus* NAD synthetase or NAD synthetase-like substrate binding pocket, the substrate binding pocket comprising the amino acids listed in Table 3;

supplying the computer modeling application with a set of structure coordinates for a chemical entity;

evaluating the potential binding interactions between the chemical entity and substrate binding pocket of the molecule or molecular complex;

structurally modifying the chemical entity to yield a set of structure coordinates for a modified chemical entity; and

determining whether the modified chemical entity is an inhibitor expected to bind to or interfere with the molecule or molecular complex, wherein binding to or interfering with the molecule or molecular complex is indicative of potential inhibition of *S. aureus* NAD synthetase activity.

22. The method of claim 21 wherein the substrate binding pocket comprises the amino acids listed in Table 3, the substrate binding pocket being defined by a set of points having a root mean square deviation of less than about 1.1Å from points representing the backbone atoms of said amino acids as represented by structure coordinates listed in Table 1.

23. The method of claim 21 wherein determining whether the modified chemical entity is an inhibitor expected to bind to or interfere with the molecule or molecular complex comprises performing a fitting operation between the chemical entity and a binding pocket of the molecule or molecular complex, followed by computationally analyzing the results of the fitting operation to quantify the association between the chemical entity and the binding pocket.

24. The method of claim 21 wherein the set of structure coordinates for the chemical entity is obtained from a chemical fragment library.

25. A computer-assisted method for designing an inhibitor of *S. aureus* NAD synthetase activity *de novo* comprising:

supplying a computer modeling application with a set of structure coordinates of a molecule or molecular complex, the molecule or molecular complex comprising at least a portion of an *S. aureus* NAD synthetase or NAD synthetase-like substrate binding pocket, wherein the substrate substrate binding pocket comprises the amino acids listed in Table 3;

computationally building a chemical entity represented by set of structure coordinates; and

determining whether the chemical entity is an inhibitor expected to bind to or interfere with the molecule or molecular complex, wherein binding to or interfering with the molecule or molecular complex is indicative of potential inhibition of *S. aureus* NAD synthetase activity.

26. The method of claim 25 wherein the substrate binding pocket comprises the amino acids listed in Table 3, the substrate binding pocket being defined by a set of points having a root mean square deviation of less than about 1.1Å from points representing the backbone atoms of said amino acids as represented by structure coordinates listed in Table 1.

27. The method of claim 25 wherein determining whether the chemical entity is an inhibitor expected to bind to or interfere with the molecule or molecular complex comprises performing a fitting operation between the chemical entity and a binding pocket of the molecule or molecular complex, followed by computationally analyzing the results of the fitting operation to quantify the association between the chemical entity and the binding pocket.

28. The method of any of claims 17, 21, or 25 further comprising supplying or synthesizing the potential inhibitor, then assaying the potential inhibitor to determine whether it inhibits *S. aureus* NadE activity.

29. A method for making an inhibitor of *S. aureus* NadE activity, the method comprising chemically or enzymatically synthesizing a chemical entity to yield an inhibitor of *S. aureus* NadE activity, the chemical entity having been identified during a computer-assisted process comprising supplying a computer modeling application with a set of structure coordinates of a molecule or molecular complex, the molecule or molecular complex comprising at least a portion of at least one of a *S. aureus* NAD synthetase or NAD synthetase-like substrate binding pocket; supplying the computer modeling application with a set of structure coordinates of a chemical entity; and determining whether the chemical entity is expected to bind to or interfere with the molecule or molecular complex at a binding pocket, wherein binding to or interfering with the molecule or molecular complex is indicative of potential inhibition of *S. aureus* NadE activity.

30. A method for making an inhibitor of *S. aureus* NadE activity, the method comprising chemically or enzymatically synthesizing a chemical entity to yield an inhibitor of *S. aureus* NadE activity, the chemical entity having been designed during a computer-assisted process comprising supplying a computer modeling application with a set of structure coordinates of a molecule or molecular complex, the molecule or molecular complex comprising at least a portion of at least one of a *S. aureus* NAD synthetase or NAD synthetase-like substrate binding pocket; supplying the computer modeling application with a set of structure coordinates for a chemical entity; evaluating the potential binding interactions between the chemical entity and a binding pocket of the molecule or molecular complex; structurally modifying the chemical entity to yield a set of structure coordinates for a modified chemical entity; and determining whether the chemical entity is expected to bind to or interfere with the molecule or molecular complex at the binding pocket, wherein binding to or interfering with the molecule or molecular complex is indicative of potential inhibition of *S. aureus* NadE activity.

31. A method for making an inhibitor of *S. aureus* NadE activity, the method comprising chemically or enzymatically synthesizing a chemical entity to yield an inhibitor of *S. aureus* NadE activity, the chemical entity having been designed during a computer-assisted process

comprising supplying a computer modeling application with a set of structure coordinates of a molecule or molecular complex, the molecule or molecular complex comprising at least a portion of at least one of a *S. aureus* NAD synthetase or NAD synthetase-like substrate binding pocket; computationally building a chemical entity represented by set of structure coordinates; and determining whether the chemical entity is expected to bind to or interfere with the molecule or molecular complex at a binding pocket, wherein binding to or interfering with the molecule or molecular complex is indicative of potential inhibition of *S. aureus* NadE activity.

32. An inhibitor of *S. aureus* NAD synthetase activity identified, designed or made according to the method of any of the claims 17, 21, 25, 29, 30, and 31.

33. A composition comprising an inhibitor of *S. aureus* NAD synthetase activity identified or designed according to the method of any of the claims 17, 21, 25, 29, 30, and 31.

34. A pharmaceutical composition comprising an inhibitor of *S. aureus* NAD synthetase activity identified or designed according to the method of any of the claims 17, 21, 25, 29, 30, and 31 or a salt thereof, and pharmaceutically acceptable carrier.

35. A method for crystallizing an *S. aureus* NAD synthetase molecule or molecular complex comprising:

providing purified *S. aureus* NAD synthetase at a concentration of about 1 mg/ml to about 50 mg/ml; and

crystallizing *S. aureus* NAD synthetase from a solution comprising about 5% by weight to about 50% by weight PEG and about 0% by weight to about 20% by weight DMSO.

36. A method for crystallizing an *S. aureus* NAD synthetase molecule or molecular complex comprising:

providing purified *S. aureus* NAD synthetase at a concentration of about 1 mg/ml to about 50 mg/ml; and

crystallizing *S. aureus* NAD synthetase from a solution comprising about 1% by weight to about 10% by weight PEG, about 0.1 M to about 5 M ammonium sulfate, and about 0% by weight to about 20% by weight DMSO, wherein the solution is buffered to a pH of about 6 to about 9.

37. A method for crystallizing an *S. aureus* NAD synthetase molecule or molecular complex comprising:

providing purified *S. aureus* NAD synthetase at a concentration of about 1 mg/ml to about 50 mg/ml; and

crystallizing *S. aureus* NAD synthetase from a solution comprising about 5% by weight to about 50% by weight PEG and about 0% by weight to about 20% by weight DMSO, wherein the solution is buffered to a pH of about 8 to about 11.

38. A crystal of *S. aureus* NAD synthetase.

39. The crystal of claim 38 having the trigonal space group symmetry $P2_1$.

40. The crystal of claim 38 comprising a unit cell having dimensions of a, b, and c; wherein a is about 40Å to about 60Å, b is about 90Å to about 120Å, and c is about 80Å to about 110Å; and wherein $\alpha = \gamma = 90°$ and β is about 80° to about 120°.

41. The crystal of claim 38 comprising atoms arranged in a spatial relationship represented by the structure coordinates listed in Table 1.

42. The crystal of claim 38 having amino acid sequence SEQ ID NO:1.

43. The crystal of claim 38 having amino acid sequence SEQ ID NO:1, with the proviso that at least one methionine is replaced with selenomethionine.